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ARMSTRONG LABORATORY

JP-8 COMPOSITION AND VARIABILITY

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This report is intended to provide information on the chemical composition of JP-8 fuel for use in assessing the impact of this fuel's use. The composition information contained in this report was obtained from a snapshot sampling of JP-8 fuel in use worldwide. Although it was not possible to obtain samples from all JP-8 locations, the samples obtained from regional aerospace fuels laboratories in Italy, Tampa, FL., Dayton, OH, and Mukilteo, WA are expected to include coverage of most worldwide suppliers of this type of fuel. The fuel samples were analyzed by gas chromatography/mass spectrometry using a medium high resolution gas chromatographic separation. A large number of the hydrocarbon components in the samples were identified and quantitated using a target compound analysis scheme which combined gas chromatographic and mass spectral information in an effort to ensure the correct compounds were quantitated and that interferences from co-eluting compounds were minimized. In addition to this careful attemp at quantifying most of the hydrocarbon constituents of the fuel, the raw chromatographic peak areas of the total ion chromatograms were examined, and the components responsible for the 100 peaks with the largest average areas were tentatively identified from the mass spectral data

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PREFACE

This report was prepared by the Armstrong Laboratory, Environics Directorate, Environmental Research Division (AL/EQC), 139 Barnes Drive, Suite 2, Tyndall AFB, FL 32403-5323.

This report was prepared in response to a request for information received from ACC/LGCO and AMC/CEMC on the composition of JP-8 jet fuel to be used in preparing Title V permit applications. These requests for information prompted AL/EQC to obtain a sampling of JP-8 fuel available in the US and abroad and to analyze the samples in detail for their organic chemical composition. This report is being made generally available.

The work was performed between August 1994 and February 1995 in house by the Armstrong Laboratory, Environics Directorate, Environmental Research Division.

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EXECUTIVE SUMMARY

This report is intended to provide information on the chemical composition of JP-8 fuel for use in assessing the impact of this fuel's use. The composition information contained in this report was obtained from a snapshot sampling of JP-8 fuel in use worldwide. Although it was not possible to obtain samples from all JP-8 locations, the samples obtained from regional aerospace fuels laboratories in Italy, Tampa, FL., Dayton, OH, and Mukilteo, WA are expected to include coverage of most worldwide suppliers of this type of fuel. The fuel samples were analyzed by gas chromatography/mass spectrometry using a medium high resolution gas chromatographic separation. A large number of the hydrocarbon components in the samples were identified and quantitated using a target compound analysis scheme which combined gas chromatographic and mass spectral information in an effort to ensure the correct compounds were quantitated and that interferences from co-eluting compounds were minimized. In addition to this careful attemp at quantifying most of the hydrocarbon constituents of the fuel, the raw chromatographic peak areas of the total ion chromatograms were examined, and the components responsible for the 100 peaks with the largest average areas were tentatively identified from the mass spectral data.

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COMPOSITION AND VARIABILITY OF JP-8

SECTION I

INTRODUCTION

OBJECTIVE:

This report is intended to provide information on the bulk composition of JP-8 fuel for use in environmental permitting, environmental planning, and formulating environmental impact statemensts. This information is urgently required in order for the Air Force to comply with new Environmental Protection Agency Title V requirements.

BACKGROUND:

During the 1990's, many units of the U. S. Air Force have changed their usage of fuel from JP-4, in use since the 1950's, to JP-8. JP-4, JP-8 and all other military fuels are purchased by specifications defining the physical properties of the products. These specifications permit broad variations in chemical composition. JP-4 fuel consisted of a wide-cut petroleum distillate exhibiting material from the lighter naptha fraction as well as the kerosene fraction of petroleum. JP-8 fuel complies with a set of specifications which is essentially identical with those of the civilian aviation fuel Jet-A1 except for fuel additives required by the JP-8 specification[1].

The composition of JP-4 fuel was the subject of a study undertaken jointly by the Headquarters Air Force Engineering and Services Center, Air Force Civil Engineering Laboratory and the U. S. Air Force Wright Laboratories, via contract with The Monsanto Company. This study assembled refinery samples of JP-4 from over 50 sources. Single samples of JP-5, JP-8, and shale-derived JP-4 were also examined in this study. The findings of this study were published in a three volume interim technical report and a final report[2,3].

The Environics Division of the Air Force Civil Engineering Laboratory also studied the Fate and Effect of JP-4 releases in the atmosphere, in surface waters, and in soils and groundwater. These studies concentrated on the biodegradation and evaporation characteristics of JP-4[4-6]. During the Air Force's early deliberations concerning the possible changeover of operations from the use of JP-4 to JP-8, Environics also studied the biodegradation of JP-8 released into soil and water[7, 8]. The use of JP-8 as a reserve boiler fuel for Air Force installations was jointly studied by the Environics and Energy divisions of the Air Force Engineering and Services Laboratory, focusing on operational aspects of the fuel used in boilers and on environmental emissions from a boiler using JP-8[9].

The Air Force is now in the process of changing operations at its installations within the Continental United States to use JP-8 in place of JP-4. This changeover has required the alteration of many environmental impact estimates. In addition, Air Force bases in the United States are now required to complete toxic emission inventories to estimate atmospheric emissions. These have prompted efforts to refine information about JP-8 composition and emissions. The Environics Directorate of the Armstrong Laboratory, formerly the Environics Division of the Air Force Engineering & Services Center, has responded by undertaking a study of JP-8 fuel composition in a series of samples collected from Aerospace Fuels Laboratories operated by the Defense Logistics Agency.

SCOPE:

This document describes the collection of a set of JP-8 fuel samples and their analysis to determine a portion of their composition. Aviation turbine fuels are mixtures of hydrocarbons derived from petroleum through refinement processes. These mixtures are extremely complex, exhibiting most if not all possible structural isomers for any possible hydrocarbon composition which falls within the physical property range of the product mixture. Jet fuels typically range in composition from 6-carbon hydrocarbons to 18-carbon hydrocarbons. As a result, thousands of individual hydrocarbon compounds

may be present in a jet fuel sample. An exhaustive separation and analysis of all organic compounds in a fuel is not practical due to the number and variety of hydrocarbons present and the limitations of the analytical chemistry state of the art. Thus, this effort has concentrated on identifying and quantifying the most abundant and thus most significant components of JP-8 fuel.

SECTION II

GAS CHROMATOGRAPHY/MASS SPECTROMETRY

The most detailed analysis available for jet fuel samples is obtained by separating the mixture with gas chromatographic techniques and further analyzing the separated materials with mass spectrometry. The chromatographic resolution of the fuel mixtures is controlled by the efficiency of the column, the injector, and the detector. Gas chromatographic columns are readily available which can separate between 200 and 300 peaks from jet fuel samples. Even with this degree of detail, chromatograms of jet fuels separated with such columns usually include a portion of incompletely resolved material which forms a "hump" on top of which more plentiful components are exhibited as peaks. The resolving power of a gas chromatographic column is generally considered to be measured by the number of "plates" it exhibits. The complete resolution of a jet fuel would require a column with an extremely high separating power, i.e. a high number of plates, plus an unusually long analysis time. The highest plates numbers are obtained using capillary gas chromatography columns, which are open tubes, 0.75mm or less in diameter and 5 m or more in length. Capillary columns can be made arbitrarily long, but columns longer then 100 m usually must be custom manufactured.[10]

The mass spectral detection of the separated fuel components is accomplished with a mass spectrometer coupled directly to the gas chromatograph. When capillary columns are used for the gas chromatographic separations, the columns can usually be plumbed directly into the mass spectrometer so that mass spectra are obtained immediately as the material exits the separatory column. The sample components enter the mass spectrometer in a region called an ion source. In the ion source, a portion of the material is converted from neutral molecules into ions.[11]

The most commonly used ion source type uses an electron beam to collisionally remove electrons from the sample molecules, yielding positive ions. This ion source is termed an electron impact (EI) source. The ions produced are accelerated and focused electrostatically into a mass filter, which may be a magnetic filter, a quadrupole mass filter, a simple time-of-flight tube, or other device which separates the ions on the basis of their mass-to-charge ratio. Most ionic species are un-stable, and molecular bond breaking or re-arrangements are common. The fragmentation of the ions depends upon the parent molecular structure and the energy imparted to the ion during its formation. Many of the fragment species also are charged. During operation, the ion source contains a plasma which consists of ionized molecules of the original sample plus fragment ions. The fragment ions and their abundances relative to the parent molecular ions are a reproducible phenomenon, and the mass spectrometer's record of these abundances is termed the sample's mass spectrum.[12]

A mass spectrometer coupled to a gas chromatograph can be used as a gas chromatographic detector in several ways. The effective utilization of a mass spectrometer in conjunction with a gas chromatograph requires that a computer be used to co-ordinate rapid scanning and data recording from the instruments. In most cases, the mass spectrometer is scanned rapidly and repeatedly, and the mass spectral observations are recorded in the computer's data storage system. The total of all ion intensities in a mass spectrum can be summed to yield a signal of total intensity versus time, which is termed the total ion chromatogram (TIC). Signals from selected ions can also be displayed versus time in order to enhance the detection of target analytes. Most data system computers for combined gas chromatography/mass spectrometry (GC/MS) can be used to plot total ion chromatograms or selected ion profiles. They can also be used to quantitate the chromatographic signals either from the total ion chromatograms or selected ion profiles. When peaks of interest have been located, the mass spectra of the compounds responsible for them can be retrieved from the computer and identified either through computerized mass spectral library searches or by manual spectrum interpretation.

In addition to the detection by scanning the mass spectrometer, detection can be greatly increased in sensitivity by a technique termed selective ion monitoring (SIM), in which the mass spectrometer is set for extended periods of time during each scan to detect designated ion signals, while ignoring other ion signals. The added sensitivity is obtained at the expense of sacrificing the option to identify the compounds responsible for peaks of interest in the sample's chromatogram by their mass spectra.

Identification of peaks in chromatograms obtained by SIM is still possible based on the retention time information.

The analysis of an unknown fuel mixture can be performed by using standard compound injections to assemble a library collection of chromatographic retention data and GC/MS response measurements. If possible the mass spectral identifications should be confirmed by analysis of authentic standards, and by confirming agreement of mass spectral and gas chromatographic measurements. The total ion chromatogram is a non-specific chromatographic representation of the sample. Thus the TIC plot is analagous to a flame ionization detector tracing in that all components in the sample should be represented as a peak rising above the baseline of the chromatogram at a characteristic time.

Quantitation of a compound using any chromatographic detector is based on the integrated area of the compound's peak., as is shown in Equation 1.[10]

$$c_i = \frac{A_i}{F_i} \qquad \text{Equation 1}$$

Where c_i is the concentration of compound i, A_i is the area of the compound's chromatographic peak, and F_i is a factor which is termed the compound's response factor. Prior to determining the concentrations in an unknown sample, standard samples, containing known amounts of the analytes of interest must be run so that each substances response factor can be determined. Greater accuracy can usually be had by using an internal standard, which is introduced into the gas chromatographic analysis along with the sample to be analyzed. If an internal standard is injected with a concentration c_s along with the unknown, and yields an internal standard peak of area A_s, then the concentration of the unknown i can be determined from Equation 2.[10]

$$c_i = \frac{A_i \times c_s}{A_s \times F_{is}} \qquad \text{Equation 2}$$

Where F_{is} is the internal-standardized response factor for the analyte i [10]. Whether an internal standard is used or not, a mass spectrometer can be used as a detector and can provide quantitation of the target analyte whether using the peak area of the analyte peak in a total ion chromatogram or using only a selected quantifier ion in a selected ion profile.

An alternative strategy is to analyze the unknown fuels by GC/MS and examine the total ion chromatograms for peaks, which can then be identified through mass spectral interpretation. A crude approximation of the concentration of a given compound in the fuel can be obtained by integrating the TIC peak for each compound and using the percentage of the peak's area in the TIC as the estimate for the percentage of the compound in the fuel, as is shown in Equation 3.

$$c_{j\%} \approx \frac{A_j}{\sum_{AllPeaks} A_i} \times 100\% \qquad \text{Equation 3}$$

Where $c_{j\%}$ is the weight percentage concentration of compound j, A_j is the area of the peak from compound j. This approximate treatment has the effect of assuming that all components represented in the TIC have identical reponse factors, equal to unity.

SECTION III

STATISTICS

The average concentration of each quantitated compound over the set of samples was calculated using Equation 4.

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i \qquad \text{Equation 4}$$

Where x_i is the measurement made on trial i and n is the total number of measurements made in the sampling.[13]

The standard deviation s for each compound's concentration was estimated using the computational formula for the standard deviation of a population, estimated from a sampling of the population, shown in Equation 5.[13]

$$s = \sqrt{\frac{n\sum_{i=1}^{n} x_i^2 - (\sum_{i=1}^{n} x_i)^2}{n(n-1)}} \qquad \text{Equation 5}$$

The minimum and maximum concentrations obtained for each compound were also obtained and tabulated. Confidence limits for the mean of each compound's concentration was calculated, using Student's-T distribution. The formula for the width of the confidence interval, w_c for the mean concentration of each compound can be found from Equation 6.

$$w_c = \pm \frac{t_{\alpha/2,\nu}}{\sqrt{\nu}} s \qquad \text{Equation 6}$$

Where ν is the number of degrees-of-freedom in the estimate, i,e, n-1, t is Student's t, and α is the significance level. To obtain a 95% confidence interval, α is set to 0.05. It should be noted that the widths of confidence intervals calculated with Equation 3 predict the compound mean concentrations, and not concentrations which could be obtained from future analyses of JP-8.[13]

A final statistical question which may be of interest is the question of the largest concentration of a compound which is likely to be encountered in JP-8. Consulting a table of distribution-free tolerance limits indicates that with 63 samples, 95% of the JP-8 concentration population for a given analyte should lie at values below the maximum concentration encountered.[14]

SECTION IV

PROCEDURE

Samples of fuel were obtained from the Defense Logistics Agency Regional Aerospace Fuels Laboratories at MacDill AFB, FL, Mukilteo WA, and Aviano AB, Italy as well as from the Propulsion Fuels Directorate at Wright Laboratories, Wright Patterson AFB, OH. An additional sample was available from Arnold AFB, TN which had been collected for a previous effort by the Environics Directorate of the Armstrong Laboratory. With the exception of samples from Wright Laboratories and Arnold AFB, TN, the samples were collected and stored at $0^{O}C$ in glass vials of approximately 18 mL capacity, with teflon lined plastic screw caps. The samples from Wright Laboratory's Propulsion Fuel Directorate were obtained in 1 mL crimp-on autosampler vials and stored at $-20^{O}C$ until use. The sample from Arnold AFB, TN was obtained as a bulk sample and was stored at $0^{O}C$.

Each sample was diluted with methylene chloride and spiked with d_{10}-anthracene as an internal standard prior to analysis by gas chromatography/mass spectrometry (GC/MS). For each fuel sample injection, an autosampler vial was filled with 800 µL of methylene chloride, 100 µL of the JP-8 fuel sample, and 100 µL of an internal standard solution consisting of 2.52 mg/mL d_{10}-anthracene in methylene chloride. The vial was then capped with a crimp-top lid with a teflon-faced silicone rubber septum. The methylene chloride solvent and internal standard solutions were measured for this preparation with glass gas-tight syringes equipped with luer-mounted needles. Fuel aliquots were measured by pipette (Rainen EDP-Plus, 250 µL tip, Rainin, Inc.). The vials containing the diluted samples with internal standard were analyzed by GC/MS.

The GC/MS analyses were performed with a gas chromatograph/mass selective detector system consisting of a HP-5890 gas chromatograph and a HP-5970B mass selective detector. The system was equipped with a HP-7673 autosampler for automatic injection of samples. The data system consisted of a personal computer (HP Vectra) with a 66 Mhz '486 microprocessor, 16 Mbytes of RAM, 430 Mbytes of disk storage, and a 120 Mbyte tape backup unit (Connor). The data system was operated with MS-DOS 6.22/Windows 3.11, and also operated Hewlett-Packard DOS Chemstation software and Enviroquant software.

The diluted fuel samples were introduced into the gas chromatograph via a split/splitless injection port operating in the split mode. Sample injection was via the HP-7673 autosampler using nominal injection volumes of 0.5 µL and a split flow of approximately 60 mL/min. The separations were made with a fused silica capillary column, 30 m long with an internal diameter of 0.25 mm, coated with 1 µm of 5% phenyl-substituted polymethylsiloxane (DB-5, J&W Scientific Inc.). The column oven was held isothermal at 40 ^{O}C for 4 min and then temperature programmed at 3 ^{O}C/min to 270 ^{O}C and held isothermal for 10 min.. The carrier gas was helium, supplied at a constant head pressure of 15 psig. The capillary column was interfaced to the mass selective detector via a direct inlet transfer line to the ion source

The mass selective detector was scanned from 35 to 350 daltons with a scan delay of 4 min to allow the solvent to elute prior to activating the detector. The mass selective detector was tuned prior to each data collection sequence using perfluorotributylamine (PFTBA) and Hewlett-Packard Autotune software.

In order to calibrate the analysis, it was necessary to run a number of standards of compounds suspected to be components of JP-8. To do this a collection of hydrocarbon standards was assembled and made into a standard solution in methylene chloride. This solution was mixed with the d_{10}-anthracene internal standard plus additional methylene chloride for injection in order to calibrate the analysis. In preparing the analytical method, it was necessary to identify the retention time at which each component could be expected and also identify several ions to be used by the Enviroquant software for quantitation and identification of each analyte. In preparing the method it was necessary to analyze several subsets of five to fifteen components, chosen with differing boiling points, molecular weights, and/or molecular structure so that there was minimal danger of co-elution of components in a given subset. For final preparation of the method, data from all of the components were combined and sorted by retention time to give a list of all standard components. This list, sorted by retention time, allowed the easy location of all components which would co-elute. For some of the co-eluting pairs of compounds, it was possible to

devise a unique analysis based on differing mass spectral respones for the two components. In some cases, however, neither the gas chromatographic separation nor the mass spectral data permitted an unambiguous analysis of some components. Those components found to co-elute and to be indistinguishable by mass spectra were combined so that only one entry appeared in the compound list for both components.

For final quantitation, a standard mixture of 225 components was prepared in methylene chloride. This standard mixture was prepared as a stock, with the concentrations as listed in Table 1. Note that the densities given in Table 1 are from the CRC Handbook [16]. This mixture was then diluted with methylene chloride to achieve desired concentrations for calibration injections and was spiked with the d_{10}-anthracene internal standard. The diluted calibration standards were placed in crimp-top autosampler vials for injection. For each compound in the calibration standard, a quantitation ion had been chosen plus several confirmation ions. The quantitation ion was used to form a selected ion profile in the vicinity of the compounds elution time, and if the compound was present a peak would occur within the detection window of the selected ion profile. The quantitation ion profile peaks were integrated to give a chromatographic response. In order to quantify each target compound, the quantitation ion profile peak area was ratioed with the area of a quantitation ion profile peak for d_{10}-anthracene. Confirmation ions were used by the Enviroquant software and the chemical analysis personnel to confirm that a peak occuring with an expected ion and retention time was in fact a specific analyte. Compound identifications were thus based both upon retention time and mass spectral response.

Table 1. Preparation of Quantitation Stock Solution.

Compound	Volume	Density	Weight	Conc.	Retention Time	Quantifier Ion
--	(µL)	(g/mL)	(mg)	(mg/mL)	(min)	(amu)
2,3,3-trimethyl-1-butene	25.0	0.7050	17.63	1.763	4.30	55
2,2,3-trimethylbutane	25.0	0.6901	17.25	1.725	4.31	57
3,3-dimethylpentane	25.0	0.6936	17.34	1.734	4.90	43
benzene	25.0	0.8787	21.97	2.197	5.19	78
2-methylhexane	25.0	0.6787	16.97	1.697	5.31	43
3-ethylpentane	25.0	0.6982	17.46	1.746	6.05	43
t-1,3-dimethylcyclopentane	25.0	0.7443	18.61	1.861	6.09	70
iso-octane	25.0	0.6919	17.30	1.730	6.11	57
1-heptene	25.0	0.6970	17.43	1.743	6.24	41
n-heptane	25.0	0.6838	17.09	1.709	6.60	43
3-heptene	25.0	0.7030	17.58	1.758	6.61	41
2,2-dimethylhexane	25.0	0.6953	17.38	1.738	7.53	57
1,1,3-trimethylcyclopentane	25.0	0.7439	18.60	1.860	7.68	55
2,3,3-trimethyl-1,4-pentadiene	25.0	0.7990	19.98	1.998	7.69	95
2,4,4-trimethyl-2-pentene	25.0	0.7218	18.05	1.805	7.90	97
2,5-dimethylhexane	25.0	0.6935	17.34	1.734	7.90	97
3,3,5,5-tetramethylcyclopentene	25.0	0.7620	19.05	1.905	7.95	109
2,4-dimethylhexane	25.0	0.6960	17.40	1.740	8.10	43
3,3-dimethylhexane	25.0	0.7100	17.75	1.775	8.46	43
4-methylcyclohexene	25.0	0.7991	19.98	1.998	8.48	81
c,t,c-1,2,3-trimethylcyclopentane	25.0	0.7535	18.84	1.884	8.85	55
2,3,4-trimethylpentane	25.0	0.7191	17.98	1.798	8.93	43
2,3,3-trimethylpentane	25.0	0.7262	18.16	1.816	9.16	43
t-3,4,4-trimethyl-2-pentene	25.0	0.7390	18.48	1.848	9.35	
1,1,3,3-tetramethylcyclopentane	25.0	0.7512	18.78	1.878	9.67	111
2-methylheptane	25.0	0.6980	17.45	1.745	9.73	43
methylbenzene (toluene)	25.0	0.8669	21.67	2.167	9.80	91
4-methylheptane	25.0	0.7046	17.62	1.762	9.82	43
2,2,4,4-tetramethylpentane	25.0	0.7195	17.99	1.799	10.15	57
3-methylheptane	25.0	0.7058	17.65	1.765	10.18	43
3-ethylhexane	25.0	0.7136	17.84	1.784	10.19	43
t-1,1,3,4-tetramethylcyclopentane	25.0	0.7420	18.55	1.855	10.21	69
c-1,3-dimethylcyclohexane	25.0	0.7660	19.15	1.915	10.43	97
2-ethyl-1-hexene	25.0	0.7330	18.33	1.833	11.01	70
2,2,4-trimethylhexane	25.0	0.7110	17.78	1.778	11.05	57
1-ethyl-1-methylcyclopentane	25.0	0.7767	19.42	1.942	11.33	83
n-octane	25.0	0.7025	17.56	1.756	11.59	43
c,t,c-1,2,3,4-tetramethylcyclopentane	25.0	0.7390	18.48	1.848	11.65	69
c,c,c-1,2,3-trimethylcyclopentane	25.0	0.7792	19.48	1.948	11.80	70
c-1,4-dimethylcyclohexane	25.0	0.7829	19.57	1.957	11.91	97
t-1,3-dimethylcyclohexane	25.0	0.7847	19.62	1.962	11.91	97
2,4,4-trimethylhexane	25.0	0.7201	18.00	1.800	11.96	43
1,2,3-trimethylcyclopentene	25.0	0.8039	20.10	2.010	12.18	95
1,2,4,4-tetramethylcyclopentene	25.0	0.8000	20.00	2.000	12.35	109
c-1,1,3,4-tetramethylcyclopentane	25.0	0.7400	18.50	1.850	12.37	69
(c&t)-2,2,4-trimethyl-3-hexene	25.0	0.7520	18.80	1.880	12.52	69

Table 1. Preparation of Quantitation Stock Solution. (Continued)

Compound	Volume	Density	Weight	Conc.	Retention Time	Quantifier Ion
--	(µL)	(g/mL)	(mg)	(mg/mL)	(min)	(amu)
2-octene (cis?)	25.0	0.7240	18.10	1.810	12.53	41
2,4-dimethylheptane	25.0	0.7115	17.79	1.779	12.86	43
2,2,3-trimethylhexane	25.0	0.7257	18.14	1.814	12.92	57
2,3,3-trimethyl-1-hexene	25.0	0.7600	19.00	1.900	12.97	83
3,3,5-trimethylcyclohexene	25.0	0.7888	19.72	1.972	12.98	67
4,4-dimethylheptane	25.0	0.7221	18.05	1.805	13.01	43
2,6-dimethylheptane	25.0	0.7089	17.72	1.772	13.23	43
c-1,2-dimethylcyclohexane	25.0	0.7963	19.91	1.991	13.28	55
2,2,5,5-tetramethylhexane	25.0	0.7187	17.97	1.797	13.32	57
propylcyclopentane	25.0	0.7763	19.41	1.941	13.41	69
c,c,c-1,3,5-trimethylcyclohexane	25.0	0.7699	19.25	1.925	13.42	69
1,3,5-trimethylcyclohexane	25.0	0.7700	19.25	1.925	13.42	69
2,4,4-trimethyl-1-hexene	25.0	0.7420	18.55	1.855	13.44	43
ethylcyclohexane	25.0	0.7880	19.70	1.970	13.54	83
3,5,5-trimethylcyclohexene	25.0	0.7941	19.85	1.985	13.57	68
3,3- or 2,5-dimethylheptane	25.0	0.7226	18.07	1.807	13.63	57
2,4-dimethyl-3-ethylpentane	25.0	0.6970	17.43	1.743	13.72	43
1,1,4-trimethylcyclohexane	25.0	0.7685	19.21	1.921	13.87	111
2,3,4-trimethylhexane	25.0	0.7392	18.48	1.848	14.36	43
2,2,3,3-tetramethylpentane	25.0	0.7566	18.92	1.892	14.39	57
2,3,3,4-tetramethylpentane	25.0	0.7547	18.87	1.887	14.78	43
c,c,t-1,3,5-trimethylcyclohexane	25.0	0.7817	19.54	1.954	14.81	69
2,3-dimethylheptane	25.0	0.7260	18.15	1.815	14.84	43
3,4-dimethylheptane	25.0	0.7310	18.28	1.828	15.01	43
4-ethylheptane	25.0	0.7270	18.18	1.818	15.12	43
ethylbenzene	25.0	0.8670	21.68	2.168	15.13	91
4-methyloctane	25.0	0.7199	18.00	1.800	15.30	43
2,2-dimethylheptane	25.0	0.7105	17.76	1.776	15.30	
p-xylene	25.0	0.8611	21.53	2.153	15.63	91
3-methyloctane	25.0	0.7160	17.90	1.790	15.76	57
2,4,6-trimethylheptane	25.0	0.7190	17.98	1.798	15.91	43
c,t,t-1,2,4-trimethylcyclohexane	25.0	0.7870	19.68	1.968	16.01	69
3,3-diethylpentane	25.0	0.7500	18.75	1.875	16.02	57
2,3,3- or 3,4,4*-trimethylcyclohexene *cpd data	25.0	0.8159	20.40	2.040	16.22	68
c-1,1,3,5-tetramethylcyclohexane	25.0	0.7813	19.53	1.953	16.52	69
1-ethyl-3-methylcyclohexane	25.0	0.8094	20.24	2.024	16.74	97
1-nonene	25.0	0.7253	18.13	1.813	16.90	41
o-xylene	25.0	0.8802	22.01	2.201	17.01	91
4-nonene	25.0	0.7318	18.30	1.830	17.19	55
n-nonane	25.0	0.7176	17.94	1.794	17.43	43
c,c,t-1,2,3-trimethylcyclohexane	25.0	0.8029	20.07	2.007	17.79	55
c,c,c-1,2,3-trimethylcyclohexane	25.0	0.8027	20.07	2.007	17.81	55
c,c,c-1,2,3-trimethylcyclohexane	25.0	0.8027	20.07	2.007	17.81	55
3,3,5-trimethylheptane	25.0	0.7428	18.57	1.857	18.00	71
1-ethyl-1-methylcyclohexane	25.0	0.8090	20.23	2.023	18.10	97
1,3,5,5-tetramethyl-1,3-cyclohexadiene	25.0	0.7960	19.90	1.990	18.11	121
t-1,1,3,5-tetramethylcyclohexane	25.0	0.7900	19.75	1.975	18.29	125

Table 1. Preparation of Quantitation Stock Solution. (Continued)

Compound	Volume	Density	Weight	Conc.	Retention Time	Quantifier Ion
--	(µL)	(g/mL)	(mg)	(mg/mL)	(min)	(amu)
2,2-dimethyloctane	25.0	0.7200	18.00	1.800	18.47	57
4,4-dimethyloctane	25.0	0.7312	18.28	1.828	18.65	99
2,2,6,6-tetramethylheptane	25.0	0.7080	17.70	1.770	18.67	57
isopropylcyclohexane	25.0	0.8023	20.06	2.006	18.69	82
isopropylbenzene	25.0	0.8618	21.55	2.155	18.91	105
3,5-dimethyloctane	25.0	0.7360	18.40	1.840	18.94	57
2,7-dimethyloctane	25.0	0.7240	18.10	1.810	19.16	43
n-propylcyclohexane	25.0	0.7936	19.84	1.984	19.29	83
2,6-dimethyloctane	25.0	0.7330	18.33	1.833	19.45	71
3,4-diethylhexane	25.0	0.7472	18.68	1.868	19.79	43
3,6-dimethyloctane	25.0	0.7630	19.08	1.908	19.91	57
3,6-dimethyloctane	25.0	0.7630	19.08	1.908	19.91	57
3-ethyl-2-methylheptane	25.0	0.7398	18.50	1.850	19.91	57
3,4,5-trimethylheptane	25.0	0.7590	18.98	1.898	20.04	121
3-ethyl-3-methylheptane	25.0	0.7500	18.75	1.875	20.33	43
1,2,3,5-tetramethylcyclohexane(M.I.)	25.0	0.7790	19.48	1.948	20.65	69
propylbenzene	25.0	0.8620	21.55	2.155	20.65	91
2,3-dimethyloctane	25.0	0.7377	18.44	1.844	20.71	57
4-ethyloctane	25.0	0.7343	18.36	1.836	20.71	57
5-methylnonane	25.0	0.7326	18.32	1.832	21.00	43
4-methylnonane	25.0	0.7300	18.25	1.825	21.10	57
1-ethyl-3-methylbenzene	25.0	0.7253	18.13	1.813	21.12	105
1,3,5-trimethylbenzene	25.0	0.8652	21.63	2.163	21.12	105
1-ethyl-4-methylbenzene	25.0	0.8614	21.54	2.154	21.21	105
3-ethyloctane	25.0	0.7359	18.40	1.840	21.46	43
3-methylnonane	25.0	0.7354	18.39	1.839	21.64	57
1-ethyl-2-methylbenzene	25.0	0.8807	22.02	2.202	22.21	105
1-decene	25.0	0.7408	18.52	1.852	22.82	41
2,2,4,6,6-pentamethylheptane	25.0	0.7463	18.66	1.866	22.88	57
1-isopropyl-4-methylcyclohexane	25.0	0.7970	19.93	1.993	22.91	55
t-butylbenzene	25.0	0.8665	21.66	2.166	22.98	119
1,2,4-trimethylbenzene	25.0	0.8758	21.90	2.190	23.02	105
n-decane	25.0	0.7300	18.25	1.825	23.33	43
isobutylbenzene	25.0	0.7200	18.00	1.800	23.85	91
sec-butylbenzene	25.0	0.8621	21.55	2.155	24.04	105
3,7,7-trimethylbicyclo(4.1.0)-3-heptene	25.0	0.8570	21.43	2.143	24.07	93
1-isopropyl-3-methylbenzene	25.0	0.8610	21.53	2.153	24.66	119
1,2,3-trimethylbenzene	25.0	0.8944	22.36	2.236	24.73	105
1-ethyl-2,5-dimethylbenzene	25.0	0.8864	22.16	2.216	24.82	119
endo-dicyclopentadiene	25.0	0.9302	23.26	2.326	25.05	66
butylcyclohexane	25.0	0.7992	19.98	1.998	25.29	55
indane (2,3-dihydro-1H-indene)	25.0	0.9639	24.10	2.410	25.52	TIC
1-isopropyl-2-methylbenzene	25.0	0.8766	21.92	2.192	25.64	119
iH-indene	25.0	0.9960	24.90	2.490	26.00	115
1,3-diethylbenzene	25.0	0.8602	21.51	2.151	26.25	119
1-propyl-4-methylbenzene	25.0	0.8584	21.46	2.146	26.57	105
1,4-diethylbenzene	25.0	0.8620	21.55	2.155	26.61	119

Table 1. Preparation of Quantitation Stock Solution. (Continued)

Compound	Volume	Density	Weight	Conc.	Retention Time	Quantifier Ion
---	(μL)	(g/mL)	(mg)	(mg/mL)	(min)	(amu)
butylbenzene	25.0	0.8601	21.50	2.150	26.64	91
1-ethyl-3,5-dimethylbenzene	25.0	0.8648	21.62	2.162	26.75	119
4-methyldecane	25.0	0.7422	18.56	1.856	26.80	43
1,2-diethylbenzene	25.0	0.8800	22.00	2.200	26.96	105
2-methyldecane	25.0	0.7368	18.42	1.842	27.00	43
neopentylbenzene	25.0	0.8581	21.45	2.145	27.08	92
3-ethylnonane	25.0	0.7300	18.25	1.825	27.15	43
1-propyl-2-methylbenzene	25.0	0.8697	21.74	2.174	27.27	105
3-methyldecane	25.0	0.7420	18.55	1.855	27.37	57
1-isopropyl-4-methylbenzene	25.0	0.8573	21.43	2.143	27.83	119
1-ethyl-2,4-dimethylbenzene	25.0	0.8723	21.81	2.181	27.91	119
(1,2-dimethylpropyl-)-benzene	25.0	0.8700	21.75	2.175	28.28	105
1-ethyl-3,4-dimethylbenzene	25.0	0.8706	21.77	2.177	28.30	119
(1-ethylpropyl-)-benzene	25.0	0.8649	21.62	2.162	28.36	91
1-t-butyl-3-methylbenzene	25.0	0.8657	21.64	2.164	28.37	133
1-undecene	25.0	0.7503	18.76	1.876	28.50	41
2-ethyl-1,3-dimethylbenzene	25.0	0.8864	22.16	2.216	28.69	119
t-pentylbenzene	25.0	0.8580	21.45	2.145	28.71	119
n-undecane	25.0	0.7402	18.50	1.850	28.99	43
sec-pentylbenzene	25.0	0.8594	21.49	2.149	29.28	105
1-ethyl-3-isopropylbenzene	25.0	0.8590	21.48	2.148	29.33	133
1,2-dimethyl-3-ethylbenzene	25.0	0.8881	22.20	2.220	29.50	119
2,6-dimethyldecane	25.0	0.9000	22.50	2.250	29.96	43
1,2,4,5-tetramethylbenzene	25.0	solid	24.87	2.487	30.03	119
(2-methylbutyl-)-benzene	25.0	0.8584	21.46	2.146	30.10	92
1,2,3,5-tetramethylbenzene	25.0	0.8903	22.26	2.226	30.17	119
(3-methylbutyl-)-benzene	25.0	0.8558	21.40	2.140	30.32	92
1-t-butyl-2-methylbenzene	25.0	0.8650	21.63	2.163	31.02	133
1,2-diisopropylbenzene	25.0	0.8559	21.40	2.140	31.99	147
n-pentylbenzene	25.0	0.8585	21.46	2.146	31.99	91
1,2,3,4-tetramethylbenzene	25.0	0.9052	22.63	2.263	32.05	119
2-methylundecane	25.0	0.7480	18.70	1.870	32.43	43
4,4-dipropylheptane	25.0	0.9000	22.50	2.250	33.01	57
1,4-diisopropylbenzene	25.0	0.8568	21.42	2.142	33.10	147
1-t-butyl-3,5-dimethylbenzene	25.0	0.8500	21.25	2.125	33.24	147
1,3,3-trimethylindene	25.0	0.9370	23.43	2.343	33.25	143
1-t-butyl-4-ethylbenzene	25.0	0.8870	22.18	2.218	33.55	147
naphthalene		solid	25.19	2.519	33.82	128
1-dodecene	25.0	0.7584	18.96	1.896	33.87	41
n-dodecane	25.0	0.7487	18.72	1.872	34.31	43
(2-methylpentyl-)-benzene	25.0	0.8470	21.18	2.118	34.82	92
2,6-dimethylundecane	25.0	0.8900	22.25	2.225	35.04	57
2,2,3-trimethyldecane	25.0	0.7500	18.75	1.875	35.20	57
1,3,5-triethylbenzene	25.0	0.7310	18.28	1.828	35.60	133
n-hexylbenzene	25.0	0.8570	21.43	2.143	37.52	91
1-tridecene	25.0	0.7310	18.28	1.828	38.91	41
(1,1-diethylpropyl-)-benzene	25.0	0.9000	22.50	2.250	39.29	91
n-tridecane	25.0	0.7564	18.91	1.891	39.32	43
2-methylnaphthalene	25.0	solid	25.18	2.518	39.49	142

Table 1. Preparation of Quantitation Stock Solution. (Continued)

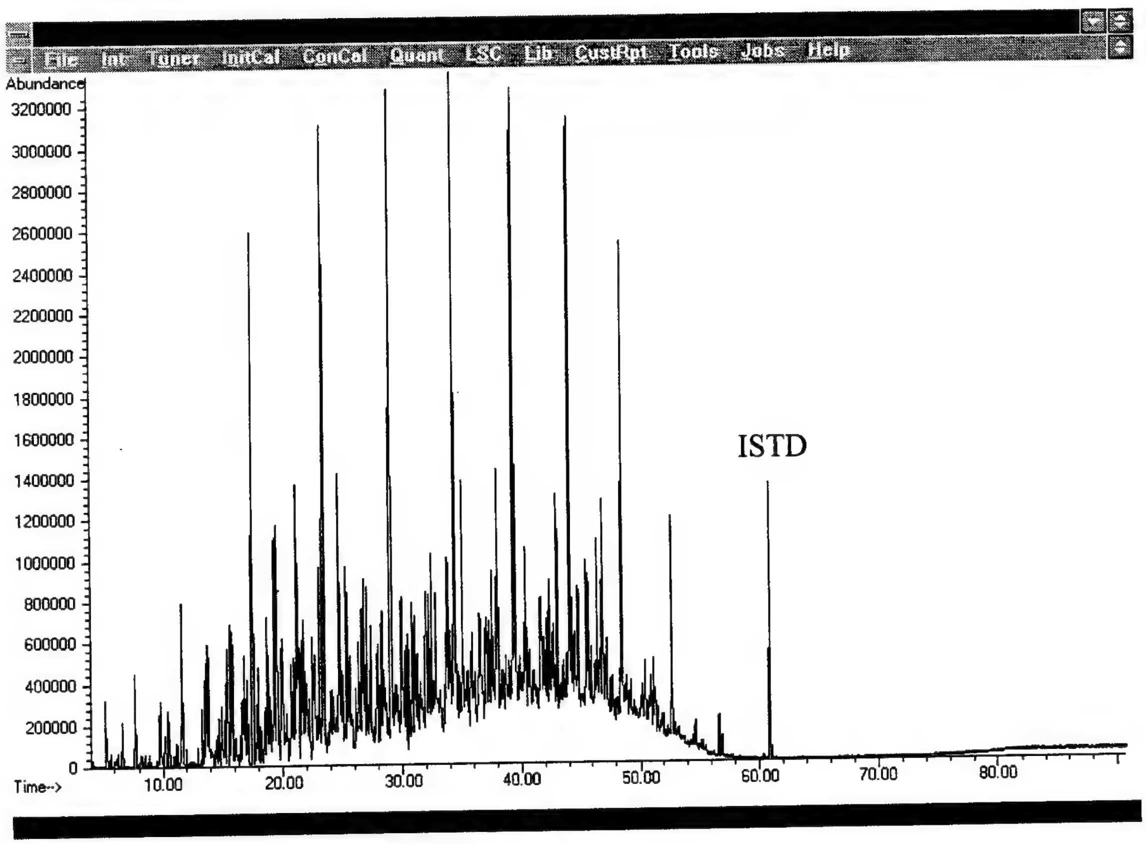
Compound	***Volume***	***Density***	***Weight***	***Conc.***	***Retention Time***	***Quantifier Ion***
--	(µL)	(g/mL)	(mg)	(mg/mL)	(min)	(amu)
1-methylnaphthalene	25.0	1.0202	25.51	2.551	40.36	141
cyclohexylbenzene	25.0	0.9502	23.76	2.376	40.72	104
1-t-butyl-3,4,5-trimethylbenze	25.0	0.8850	22.13	2.213	40.74	161
cyclododecane	25.0	solid	25.05	2.505	41.12	41
1,3,5-triisopropylbenzene	25.0	0.8450	21.13	2.113	41.23	189
heptylcyclohexane	25.0	0.7564	18.91	1.891	41.61	83
3,7,11-trimethyl-1-dodecene	25.0	0.8050	20.13	2.013	41.90	55
1,1,6-trimethyltetralin	25.0	0.9690	24.23	2.423	42.53	159
n-heptylbenzene	25.0	0.8567	21.42	2.142	42.53	91
2,6,11-trimethyldodecane	25.0	0.7980	19.95	1.995	42.77	57
2,6,10-trimethyldodecane	25.0	0.7710	19.28	1.928	42.95	57
1,1'-biphenyl	25.0	solid	25.17	2.517	43.50	154
1-tetradecene	25.0	0.7745	19.36	1.936	43.66	41
n-tetradecane	25.0	0.7628	19.07	1.907	44.02	43
2-ethylnaphthalene	25.0	0.9922	24.81	2.481	44.25	141
1-ethylnaphthalene	25.0	0.7564	18.91	1.891	44.44	141
2,6-dimethylnaphthalene	25.0	solid	25.13	2.513	44.74	156
2,3-dimethylnaphthalene	25.0	solid	25.23	2.523	46.56	141
1,4-dimethylnaphthalene	25.0	1.0166	25.42	2.542	46.56	141
1,5-dimethylnaphthalene		solid	24.98	2.498	46.56	156
1,2-dimethylnaphthalene	25.0	1.0179	25.45	2.545	47.11	141
n-octylbenzene	25.0	1.0166	25.42	2.542	47.25	92
1,8-dimethylnaphthalene		solid	25.04	2.504	48.05	156
n-pentadecane	25.0	0.7685	19.21	1.921	48.46	57
5,5-dibutylnonane	25.0	0.8240	20.60	2.060	48.86	57
n-nonylbenzene	25.0	0.8580	21.45	2.145	51.70	92
1-hexadecene	25.0	0.7811	19.53	1.953	52.34	41
n-hexadecane	25.0	0.7443	18.61	1.861	52.64	57
fluorene	25.0	solid	25.23	2.523	52.72	166
n-decylbenzene	25.0	0.8555	21.39	2.139	55.90	92
1,4,6,7-tetramethylnaphthalene		solid	25.25	2.525	56.82	184
2,6,10,14-tetramethylpentadecane	25.0	0.7830	19.58	1.958	56.88	57
hexaethylbenzene	25.0	solid	25.14	2.514	57.23	231
2,6,11,15-tetramethylhexadecane	25.0	0.7864	19.66	1.966	60.68	57
9-methylanthracene	25.0	solid	25.13	2.513	67.19	192
1-phenyltridecane	25.0	0.8550	21.38	2.138	67.27	92
pyrene		solid	25.29	2.529	72.50	202

SECTION V

RESULTS

Aerospace Fuels Laboratories and the Petroleum Fuels Directorate at Wright Laboratories provided 63 samples of JP-8 fuels. These samples were collected from widely varying regions, summarized in Table 2. GC/MS analyses were run on each of the samples. The total ion profile obtained from a typical JP-8 sample is shown in Figure 1. The peaks exhibited in this chromatogram are mainly produced by hydrocarbon compounds containing between 6 and 18 carbon atoms. The quantitative results from these GC/MS analyses are summarized in Table 3. Each compound included in the quantitative analysis scheme is listed in a row of Table 3, giving the compound name, the mean concentration in mg of component per liter of fuel, the standard deviation, and the minimum and maximum concentrations in mg/L. Note from the section on statistics that the maximum concentration found for a given compound in JP-8 serves as an estimate for maximum concentration of the compound which could be expected in JP-8.

Figure 1. Total Ion Chromatogram of a typical JP-8 sample. The peak labelled "ISTD" is the internal standard.



In addition to the directed search for the 226 target compounds, the total ion chromatograms of the 63 fuel samples were examined in an effort to gain tentative identification of the compounds responsible for the greatest proportion of the fuels' chromatograms. The total ion chromatograms were integrated, and peaks responsible for peak areas greater than one percent of the largest peak were included in an integration report. The peak retention times were converted into kovat's indices in order to reduce run-to-run retention variations. The retention indices of the integration reports' peaks were used to sort the peak integration reports into a data matrix such that each row vector of the matrix expressed the data from a single chromatogram in the data set, and each column vector of the matrix represented a single compound or co-eluting set of compounds, as recognized by the retention indices. The resulting data matrix contained 63 rows, representing the 63 samples, and 202 columns, representing 202 peaks which were found to occur at least once in the set of chromatograms. The column vectors, representing peaks in the data matrix, are also termed features.

The TIC area data vectors were entered into the MATLAB [16] matrix calculation system, and the mean, maximum, and minimum percentage area of each feature was calculated. Also, MATLAB was used to locate the run number where the maximum percentage area occured for each of the 202 features. Finally, the largest 100 features, in terms of average percentage area, were located, in terms of their feature numbers and their peak retention times. The peaks responsible were examined in the GC/MS runs where these features occured with maximum intensity. The apex mass spectrum from each peak was submitted to a computerized library search, and tentative identifications were based on the library search results. In terms of average percentage area, these 100 largest features accounted for over 94% of the area of the TIC features. These features are summarized in Table 4.

Table 2. Fuel Sample Sources.

Sample No.	*Sample Code*	*Contributing Laboratory*	*Sample Source to Laboratory*
1	94-F-2019	Mukilteo AFL	354 Supply/LGSFI Eielson AFB AK
2	94-F-2030	Mukilteo AFL	650 SUPS/LGSF Edwards AFB CA
3	94-F-2052	Mukilteo AFL	US Army AV TECH TEST CTR Edwards AFB CA
4	94-F-2284	Mukilteo AFL	US Army AV TECH TEST CTR Edwards AFB CA
5	94-F-2169	Mukilteo AFL	US Army AV TECH TEST CTR Edwards AFB CA
6	94-F-1185	MacDill AFL	Standard Transpipe Corp. Moody AFB GA
7	94-F-1095	MacDill	Continental Services Co. Hanahan SC
8	94-F-1076	MacDill	LL&E Petroleum Marketing Hurlbert Field FL
9	94-F-1241	MacDill	LL&E Petroleum Marketing Eglin AFB FL
10	94-F-1045	MacDill	K-Mar Industries MacDill AFB FL
11	94-F-1110	MacDill	Navy Supply Center Jacksonville FL
12	94-F-1164	MacDill	Gold Line Refinery Ltd. Tyndall AFB FL
13	94-F-1042	MacDill	LL&E Petroleum Marketing Eglin AFB FL
14	94-F-1249	MacDill	K-Mar Industries Clearwater FL
15	94-F-1149	MacDill	MODUK MAERSK Ascension Patrick AFB FL
16	94-F-1285	MacDill	Aviation Fuel Terminal Morehead City NC
17	94-F-1286	MacDill	Aviation Fuel Terminal Morehead City NC
18	94-F-1163	MacDill	Gold Line Refinery Ltd. Tyndall AFB FL
19	94-F-1044	MacDill	K-Mar Industries MacDill AFB FL
20	94-F-1178	MacDill	LL&E Petroleum Marketing Tyndall AFB FL
21	94-F-1159	MacDill	Aviation Fuel Terminal

Table 2. Fuel Sample Sources. (Continued)

Sample No.	*Sample Code*	*Contributing Laboratory*	*Sample Source to Laboratory*
			Morehead City NC
22	94-F-1169	MacDill	LL&E Petroleum Marketing Eglin AFB FL
23	94-F-1148	MacDill	MODUK MAERSK Ascension Patrick AFB FL
24	94-F-1161	MacDill	Aviation Fuel Terminal Morehead City NC
25	94-F-1160	MacDill	Aviation Fuel Terminal Morehead City NC
26	94-F-1078	MacDill	Eglin AFB FL
27	94-F-1237	MacDill	Robins AFB GA
28	94-F-1304	MacDill	LL&E Petroleum Marketing Tyndall AFB FL
29	94-F-1218	MacDill	Continental Services Co. Hanahan SC
30	94-F-1318	MacDill	Pratt & Whitney West Palm Beach FL
31	94-F-1167	MacDill	LL&E Petroleum Marketing Eglin AFB FL
32	94-F-1195	MacDill	LL&E Petroleum Marketing Hurlbert Field FL
33	94-F-1328	MacDill	Seymour Johnson AFB NC
34	94-F-1319	MacDill	Pratt & Whitney West Palm Beach FL
35	94-F-1302	MacDill	LL&E Petroleum Marketing Eglin AFB FL
36	94-F-1170	MacDill	LL&E Petroleum Marketing Eglin AFB FL
37	94-F-1305	MacDill	LL&E Petroleum Marketing Tyndall AFB FL
38	94-F-1308	MacDill	LL&E Petroleum Marketing Hurlbert Field FL
39	94-F-1147	MacDill	MODUK MAERSK Ascension Patrick AFB FL
40	94-F-1129	MacDill	K-Mar Industries MacDill AFB FL
41	94-F-1242	MacDill	Eglin AFB FL
42	94-F-1226	MacDill	LL&E Petroleum Marketing Eglin AFB FL
43	94-F-1109	MacDill	Shaw AFB SC
44	94-F-1032	MacDill	
45	94-F-1168	MacDill	LL&E Petroleum Marketing

Table 2. Fuel Sample Sources. (Continued)

Sample No.	*Sample Code*	*Contributing Laboratory*	*Sample Source to Laboratory*
			Eglin AFB FL
46	94-F-1219	MacDill	Continental Services Co. Hanahan SC
47	3059	Wright-Patterson	
48	2995	Wright-Patterson	San Pedro CA
49	2999	Wright-Patterson	Pearl Harbor HI
50	3001	Wright-Patterson	Anchorage AK
51	3002	Wright-Patterson	Whittier AK
52	3020	Wright-Patterson	Pearl Harbor HI
53	3047	Wright-Patterson	Pearl Harbor HI
54	3049	Wright-Patterson	Athens Gr
55	3083	Wright-Patterson	Pearl Harbor HI
56	3109	Wright-Patterson	Burlington NJ
57	3110	Wright-Patterson	Dover DE
58	89-70	Arnold AFB	Arnold AFB Tank 7
59	90-98	Aviano	Zaragoza, Spain
60	90-94	Aviano	Aviano IT, NIPS System
61	90-121F	Aviano	Union Explosives Refinery, Rio Tinto, Huelva, Spain
62	90-116	Aviano	Zaragoza, Spain
63	90-106	Aviano	Torrejon, Spain

Table 3. Summary of Target Analyte Results from JP-8.

Compound	Avg. Conc. (mg/L)	Stdev. Conc. (mg/L)	Min. Fuel (mg/L)	Max. Fuel (mg/L)
ISTD (d_{10}-anthracene)	0.00E+00	0.0E+00	0.0E+00	0.00E+00
2,2,3-trimethylbutane	1.24E+01	1.4E+01	0.0E+00	9.36E+01
2,3,3-trimethyl-1-butene	9.60E+00	7.9E+00	1.6E+00	4.31E+01
3,3-dimethylpentane	2.14E+01	3.5E+01	1.4E+00	2.44E+02
benzene	2.70E+02	6.5E+02	1.4E+00	4.95E+03
2-methylhexane	2.85E+02	3.8E+02	4.1E+00	2.71E+03
3-ethylpentane	1.90E+01	1.7E+01	1.4E+00	9.04E+01
t-1,3-dimethylcyclopentane	4.46E+01	5.2E+01	1.5E+00	2.93E+02
iso-octane	9.80E+00	7.5E+00	1.8E+00	3.59E+01
1-heptene	1.15E+02	1.4E+02	3.1E+00	8.86E+02
3-heptene	1.17E+03	9.6E+02	4.7E+00	5.83E+03
n-heptane	1.70E+03	1.4E+03	5.6E+00	8.58E+03
2,2-dimethylhexane	1.17E+01	1.8E+01	6.0E-01	1.31E+02
1,1,3-trimethylcyclopentane	2.21E+03	1.5E+03	7.6E+00	8.76E+03
2,3,3-trimethyl-1,4-pentadiene	4.20E+00	4.8E+00	0.0E+00	2.36E+01
2,4,4-trimethyl-2-pentene	6.90E+00	5.8E+00	0.0E+00	2.55E+01
3,3,5,5-tetramethylcyclopentene	7.00E-01	1.0E+00	0.0E+00	3.70E+00
2,5-dimethylhexane	6.60E+00	5.6E+00	0.0E+00	2.46E+01
2,4-dimethylhexane	1.26E+02	1.3E+02	2.7E+00	5.00E+02
3,3-dimethylhexane	5.13E+01	4.8E+01	1.7E+00	2.29E+02
4-methylcyclohexene	6.70E+00	6.1E+00	0.0E+00	2.82E+01
c,t,c-1,2,3-trimethylcyclopentane	1.92E+02	1.9E+02	1.8E+00	6.53E+02
2,3,4-trimethylpentane	2.05E+01	1.9E+01	2.1E+00	1.15E+02
2,3,3-trimethylpentane	9.20E+00	7.5E+00	1.0E+00	3.35E+01
t-3,4,4-trimethyl-2-pentene	3.90E+00	4.4E+00	0.0E+00	2.08E+01
1,1,3,3-tetramethylcyclopentane	3.80E+00	5.1E+00	0.0E+00	2.71E+01
2-methylheptane	1.49E+03	8.2E+02	3.2E+00	3.15E+03
4-methylheptane	1.05E+03	9.8E+02	8.2E+00	3.73E+03
methylbenzene (toluene)	1.75E+03	1.2E+03	9.0E-01	6.39E+03
3,4-dimethylhexane	4.65E+01	4.9E+01	2.1E+00	2.11E+02
2,2,4,4-tetramethylpentane	3.53E+02	3.1E+02	6.0E-01	1.34E+03
3-methylheptane	5.02E+02	4.8E+02	2.7E+00	1.98E+03
3-ethylhexane	6.20E+02	4.4E+02	3.2E+00	1.99E+03
t-1,1,3,4-tetramethylcyclopentane	3.53E+01	4.6E+01	2.0E+00	2.37E+02
c-1,3-dimethylcyclohexane	1.63E+03	9.8E+02	4.7E+00	4.46E+03
2-ethyl-1-hexene	2.97E+01	4.5E+01	1.4E+00	2.30E+02
2,2,4-trimethylhexane	5.50E+00	3.8E+00	4.0E-01	1.69E+01
1-ethyl-1-methylcyclopentane	2.06E+01	1.7E+01	1.7E+00	8.97E+01
c,t,c-1,2,3,4-tetramethylcyclopent	1.04E+02	1.1E+02	6.6E+00	4.91E+02
n-octane	5.05E+03	3.0E+03	4.5E+00	1.16E+04
c,c,c-1,2,3-trimethylcyclopentane	5.07E+01	1.7E+02	2.9E+00	1.15E+03
c-1,4-dimethylcyclohexane	3.27E+02	3.8E+02	1.3E+00	1.63E+03
t-1,3-dimethylcyclohexane	3.16E+02	3.7E+02	1.3E+00	1.57E+03
2,4,4-trimethylhexane	3.68E+01	5.1E+01	2.0E+00	2.81E+02
1,2,3-trimethylcyclopentene	3.00E+00	2.7E+00	0.0E+00	1.34E+01
c-1,1,3,4-tetramethylcyclopentane	6.80E+00	4.8E+00	9.0E-01	2.55E+01
1,2,4,4-tetramethylcyclopentene	1.60E+00	2.5E+00	0.0E+00	1.04E+01

Table 3. Summary of Target Analyte Results from JP-8. (Continued)

2-octene	2.75E+01	2.4E+01	2.0E+00	1.32E+02
(c&t)-2,2,4-trimethyl-3-hexene	3.22E+01	2.4E+01	3.7E+00	1.35E+02
2,4-dimethylheptane	3.56E+02	2.8E+02	1.9E+00	1.23E+03
2,2,3-trimethylhexane	4.25E+01	7.0E+01	1.4E+00	3.40E+02
2,3,3-trimethyl-1-hexene	1.82E+01	5.2E+01	1.1E+00	3.65E+02
4,4-dimethylheptane	1.41E+02	2.4E+02	1.0E+00	8.55E+02
3,3,5-trimethylcyclohexene	9.00E+00	7.6E+00	1.6E+00	3.55E+01
c-1,2-dimethylcyclohexane	4.40E+02	5.1E+02	8.9E+00	2.50E+03
2,2,5,5-tetramethylhexane	4.74E+02	4.3E+02	1.2E+00	1.69E+03
2,6-dimethylheptane	1.33E+03	8.4E+02	8.8E+01	3.76E+03
c,c,c-1,3,5-trimethylcyclohexane	1.13E+02	1.8E+02	3.1E+00	7.11E+02
c,c,t-1,3,5-trimethylcyclohexane	9.18E+01	1.7E+02	1.5E+00	9.18E+02
2,4,4-trimethyl-1-hexene	1.43E+02	5.3E+02	5.6E+00	3.26E+03
propylcyclopentane	1.18E+02	1.8E+02	2.2E+00	7.19E+02
1,3,5-trimethylcyclohexane	1.15E+02	1.8E+02	2.2E+00	7.14E+02
3,5,5-trimethylcyclohexene	6.58E+01	9.5E+01	2.8E+00	4.65E+02
ethylcyclohexane	4.15E+03	2.4E+03	2.7E+02	1.33E+04
3,3- or 2,5-dimethylheptane	1.57E+03	1.2E+03	2.9E+00	6.20E+03
2,4-dimethyl-3-ethylpentane	1.47E+02	1.9E+02	1.3E+00	8.63E+02
1,1,4-trimethylcyclohexane	1.12E+03	1.9E+03	7.0E+00	7.63E+03
2,3,4-trimethylhexane	1.14E+02	1.3E+02	4.6E+00	5.76E+02
2,2,3,3-tetramethylpentane	1.26E+01	2.2E+01	7.0E-01	1.20E+02
2,3,3,4-tetramethylpentane	1.37E+03	1.3E+03	2.4E+00	4.07E+03
2,3-dimethylheptane	1.57E+03	9.1E+02	2.3E+00	3.70E+03
3,4-dimethylheptane	5.36E+02	1.6E+03	3.1E+00	8.02E+03
4-ethylheptane	2.61E+02	4.2E+02	5.4E+00	2.65E+03
ethylbenzene	1.27E+03	7.0E+02	1.9E+01	3.63E+03
4-methyloctane	1.98E+03	1.1E+03	2.1E+00	4.76E+03
m & p-xylenes (co-eluting)	6.05E+03	3.6E+03	0.0E+00	1.53E+04
3-methyloctane	4.16E+03	1.9E+03	5.4E+02	9.01E+03
2,4,6-trimethylheptane	1.73E+02	4.6E+02	4.7E+00	2.23E+03
c-1,2,3-trimethylcyclohexane	2.05E+03	2.9E+03	1.8E+01	1.04E+04
3,3-diethylpentane	7.03E+02	1.2E+03	6.7E+00	5.15E+03
1,2,4-trimethylcyclohexane	1.86E+03	2.4E+03	3.1E+01	9.79E+03
2,3,3- or 3,4,4-trimethylcyclohexene	1.17E+01	9.5E+00	1.2E+00	5.08E+01
c,c,t-1,3,5-trimethylcyclohexane	9.18E+01	1.7E+02	1.5E+00	9.18E+02
1-ethyl-3-methylcyclohexane	2.94E+03	1.6E+03	7.1E+02	7.92E+03
1-nonene	7.12E+02	4.8E+02	2.3E+01	1.93E+03
o-xylene	3.45E+03	1.8E+03	4.6E+02	7.13E+03
4-nonene	5.64E+01	1.1E+02	4.4E+00	4.78E+02
n-nonane	1.84E+04	8.2E+03	3.9E+03	4.56E+04
c,c,t-1,2,3-trimethylcyclohexane	1.75E+02	1.3E+02	9.5E+00	5.32E+02
c,c,c-1,2,3-trimethylcyclohexane	1.13E+02	8.6E+01	6.1E+00	3.43E+02
3,3,5-trimethylheptane	4.90E+00	3.7E+00	9.0E-01	1.84E+01
1-ethyl-1-methylcyclohexane	8.40E+02	7.6E+02	8.4E+01	5.32E+03
1,3,5,5-tetramethyl-1,3-cyclohexadiene	1.30E+00	1.9E+00	0.0E+00	7.80E+00
t-1,1,3,5-tetramethylcyclohexane	1.58E+01	2.1E+01	0.0E+00	1.10E+02
2,2-dimethyloctane	5.42E+02	4.7E+02	3.7E+00	2.09E+03
2,2,6,6-tetramethylheptane	7.78E+01	1.0E+02	2.7E+00	7.21E+02

Table 3. Summary of Target Analyte Results from JP-8. (Continued)

4,4-dimethyloctane	1.15E+02	1.0E+02	9.2E+00	4.59E+02
isopropylcyclohexane	2.74E+03	1.2E+03	1.4E+01	6.36E+03
3,5-dimethyloctane	2.90E+03	3.5E+03	1.2E+01	1.51E+04
isopropylbenzene	1.45E+03	8.5E+02	0.0E+00	4.19E+03
2,7-dimethyloctane	1.84E+03	9.4E+02	4.6E+02	4.44E+03
n-propylcyclohexane	4.03E+03	1.4E+03	1.5E+03	9.07E+03
2,6-dimethyloctane	5.96E+03	2.6E+03	2.3E+01	1.55E+04
3,4-diethylhexane	3.02E+02	2.1E+02	1.6E+01	1.04E+03
3,6-dimethyloctane	2.91E+03	1.7E+03	4.6E+01	8.58E+03
3-ethyl-2-methylheptane	3.26E+03	1.8E+03	4.9E+01	9.14E+03
3,4,5-trimethylheptane	3.60E+00	4.7E+00	0.0E+00	1.82E+01
3-ethyl-3-methylheptane	5.12E+01	6.1E+01	2.4E+00	3.13E+02
1,2,3,5-tetramethylcyclohexane	1.36E+02	1.8E+02	6.9E+00	6.12E+02
propylbenzene	1.95E+03	8.9E+02	6.3E+02	5.82E+03
2,3-dimethyloctane	1.22E+03	7.0E+02	1.1E+01	3.37E+03
4-ethyloctane	1.18E+03	6.7E+02	1.1E+01	3.25E+03
5-methylnonane	1.94E+03	7.8E+02	6.2E+01	5.02E+03
4-methylnonane	6.41E+03	2.5E+03	4.9E+02	1.30E+04
1-ethyl-3-methylbenzene	3.59E+03	1.3E+03	7.5E+02	7.58E+03
1-ethyl-4-methylbenzene	3.15E+03	1.8E+03	1.7E+02	8.02E+03
3-ethyloctane	1.27E+03	1.6E+03	3.5E+02	1.28E+04
1,3,5-trimethylbenzene	4.27E+03	1.6E+03	9.0E+02	9.02E+03
3-methylnonane	6.05E+03	2.0E+03	2.5E+03	1.33E+04
1-isopropyl-4-methylcyclohexane	8.94E+01	2.3E+02	1.9E+00	1.62E+03
1-ethyl-2-methylbenzene	2.75E+03	1.1E+03	8.3E+02	7.22E+03
1-decene	2.59E+02	2.7E+02	2.3E+01	1.81E+03
2,2,4,6,6-pentamethylheptane	1.21E+01	1.8E+01	9.0E-01	9.19E+01
t-butylbenzene	1.52E+03	6.1E+02	2.0E+01	2.76E+03
1,2,4-trimethylbenzene	1.23E+04	4.3E+03	3.6E+03	2.16E+04
n-decane	3.37E+04	1.4E+04	8.1E+01	5.59E+04
isobutylbenzene	4.58E+02	2.3E+02	3.4E+00	1.02E+03
sec-butylbenzene	8.32E+02	3.8E+02	1.4E+02	1.74E+03
3,7,7-trimethylbicyclo(4.1.0)-3-heptene	1.07E+01	7.8E+00	6.0E-01	3.95E+01
1-isopropyl-3-methylbenzene	1.25E+03	4.9E+02	2.3E+02	1.95E+03
1,2,3-trimethylbenzene	5.66E+03	1.9E+03	1.4E+03	8.77E+03
1-ethyl-2,5-dimethylbenzene	1.72E+03	6.7E+02	1.0E+02	2.96E+03
dicyclopentadiene	4.30E+00	2.4E+00	6.0E-01	1.24E+01
butylcyclohexane	6.88E+03	2.9E+03	7.7E+01	1.13E+04
indane (2,3-dihydro-1H-indene)	4.05E+03	1.5E+03	1.1E+03	1.02E+04
1-isopropyl-2-methylbenzene	2.61E+02	1.6E+02	1.1E+00	6.11E+02
iH-indene	1.37E+01	2.7E+01	0.0E+00	1.31E+02
1,3-diethylbenzene	1.43E+03	5.0E+02	5.3E+02	2.75E+03
1-propyl-4-methylbenzene	1.20E+03	4.1E+02	2.8E+02	2.38E+03
1,4-diethylbenzene	6.48E+02	2.8E+02	8.9E+01	1.49E+03
butylbenzene	1.08E+03	4.2E+02	7.5E+01	2.29E+03
1-ethyl-3,5-dimethylbenzene	2.73E+03	1.0E+03	6.2E+01	4.70E+03
4-methyldecane	6.10E+03	2.0E+03	2.1E+03	1.03E+04
1,2-diethylbenzene	5.76E+02	3.5E+02	6.5E+00	1.50E+03
2-methyldecane	9.02E+03	3.9E+03	2.8E+03	1.71E+04

Table 3. Summary of Target Analyte Results from JP-8. (Continued)

neopentylbenzene	1.41E+01	1.2E+01	9.0E-01	5.07E+01
3-ethylnonane	8.06E+02	3.0E+02	2.1E+02	1.38E+03
1-propyl-2-methylbenzene	2.57E+03	1.0E+03	3.9E+02	4.54E+03
3-methyldecane	8.47E+03	3.0E+03	2.5E+03	1.42E+04
1-isopropyl-4-methylbenzene	2.10E+03	7.9E+02	3.4E+02	3.53E+03
1-ethyl-2,4-dimethylbenzene	2.68E+03	1.1E+03	7.5E+02	4.71E+03
(1,2-dimethylpropyl-)-benzene	2.60E+02	1.9E+02	1.5E+00	6.91E+02
1-ethyl-3,4-dimethylbenzene	2.14E+03	7.9E+02	0.0E+00	3.66E+03
1-t-butyl-3-methylbenzene	3.92E+01	4.1E+01	2.2E+00	1.98E+02
(1-ethylpropyl-)-benzene	3.99E+02	2.1E+02	4.5E+00	8.40E+02
1-undecene	4.90E+02	4.5E+02	2.8E+01	1.84E+03
2-ethyl-1,3-dimethylbenzene	5.05E+02	2.3E+02	2.8E+00	1.02E+03
t-pentylbenzene	4.83E+02	3.6E+02	0.0E+00	1.25E+03
n-undecane	2.88E+04	1.4E+04	7.0E+01	6.00E+04
1-ethyl-3-isopropylbenzene	3.52E+02	2.1E+02	2.1E+00	7.96E+02
sec-pentylbenzene	2.53E+02	3.0E+02	5.4E+00	1.34E+03
1,2-dimethyl-3-ethylbenzene	1.40E+03	5.3E+02	3.4E+02	2.41E+03
1,2,4,5-tetramethylbenzene	1.95E+03	9.0E+02	3.3E+01	3.85E+03
2,6-dimethyldecane	4.23E+03	2.5E+03	5.8E+01	8.66E+03
(2-methylbutyl-)-benzene	1.31E+02	1.2E+02	6.0E+00	4.74E+02
1,2,3,5-tetramethylbenzene	2.04E+03	8.8E+02	6.1E+02	3.85E+03
(3-methylbutyl-)-benzene	2.42E+02	1.5E+02	2.5E+00	6.15E+02
1-t-butyl-2-methylbenzene	4.67E+02	3.2E+02	1.9E+00	1.09E+03
1,2-diisopropylbenzene	2.22E+01	2.1E+01	0.0E+00	8.07E+01
1,2,3,4-tetramethylbenzene	1.81E+03	9.2E+02	1.8E+01	3.62E+03
n-pentylbenzene	6.21E+02	3.2E+02	2.2E+01	1.72E+03
2-methylundecane	8.22E+03	4.4E+03	7.0E+02	1.79E+04
4,4-dipropylheptane	3.38E+02	3.2E+02	2.8E+01	1.20E+03
1,4-diisopropylbenzene	1.44E+01	1.1E+01	8.0E-01	4.31E+01
1,3,3-trimethylindene	4.00E-01	6.0E-01	0.0E+00	2.70E+00
1-t-butyl-3,5-dimethylbenzene	1.72E+01	2.2E+01	1.0E+00	8.71E+01
1-t-butyl-4-ethylbenzene	6.80E+00	6.2E+00	5.0E-01	3.03E+01
naphthalene	2.14E+03	1.4E+03	2.2E+02	7.32E+03
1-dodecene	4.73E+02	7.5E+02	8.2E+00	2.76E+03
n-dodecane	2.72E+04	1.4E+04	1.2E+02	5.91E+04
(2-methylpentyl-)-benzene	2.38E+01	3.1E+01	1.3E+00	1.81E+02
2,6-dimethylundecane	1.07E+04	3.9E+03	3.6E+03	1.68E+04
2,2,3-trimethyldecane	2.67E+03	3.5E+03	2.6E+01	9.71E+03
1,3,5-triethylbenzene	5.41E+02	4.2E+02	3.1E+00	1.67E+03
n-hexylbenzene	5.50E+02	2.6E+02	6.7E+00	1.24E+03
1-tridecene	3.03E+02	2.9E+02	5.0E+00	9.97E+02
(1,1-diethylpropyl-)-benzene	2.21E+01	3.0E+01	1.3E+00	1.68E+02
n-tridecane	2.60E+04	1.1E+04	6.6E+03	4.48E+04
2-methylnaphthalene	2.98E+03	1.5E+03	0.0E+00	6.79E+03
1-methylnaphthalene	3.59E+03	1.8E+03	5.4E+02	7.97E+03
cyclohexylbenzene	3.87E+02	2.8E+02	5.2E+00	1.02E+03
1-t-butyl-3,4,5-trimethylbenzene	2.02E+01	2.8E+01	9.0E-01	1.58E+02
cyclododecane	3.95E+01	5.2E+01	4.3E+00	3.34E+02
1,3,5-triisopropylbenzene	4.00E-01	1.2E+00	0.0E+00	9.40E+00

Table 3. Summary of Target Analyte Results from JP-8. (Continued)

heptylcyclohexane	1.66E+03	6.8E+02	1.9E+00	2.77E+03
3,7,11-trimethyl-1-dodecene	3.72E+02	2.9E+02	1.5E+01	1.29E+03
1,1,6-trimethyltetralin	1.22E+02	1.2E+02	1.4E+00	5.76E+02
n-heptylbenzene	2.73E+02	1.6E+02	2.5E+00	7.70E+02
2,6,11-trimethyldodecane	1.86E+03	1.1E+03	4.1E+01	4.30E+03
2,6,10-trimethyldodecane	5.02E+03	2.3E+03	7.5E+02	9.90E+03
1,1'-biphenyl	5.42E+02	3.3E+02	1.5E+02	1.84E+03
1-tetradecene	3.67E+01	2.5E+01	5.7E+00	1.10E+02
n-tetradecane	1.68E+04	6.5E+03	1.1E+03	2.82E+04
2-ethylnaphthalene	4.55E+02	2.4E+02	1.6E+01	1.14E+03
1-ethylnaphthalene	1.19E+02	8.9E+01	3.4E+00	4.11E+02
2,6-dimethylnaphthalene	9.23E+02	6.1E+02	3.8E+00	3.28E+03
2,3-dimethylnaphthalene	1.45E+02	1.1E+02	2.9E+00	5.08E+02
1,4-dimethylnaphthalene	1.91E+02	1.4E+02	3.8E+00	6.68E+02
1,5-dimethylnaphthalene	1.94E+02	1.4E+02	3.3E+00	6.73E+02
1,2-dimethylnaphthalene	2.04E+02	1.6E+02	9.9E+00	7.19E+02
n-octylbenzene	1.09E+02	8.0E+01	4.2E+00	3.14E+02
1,8-dimethylnaphthalene	2.20E+00	2.5E+00	0.0E+00	1.10E+01
n-pentadecane	7.17E+03	2.5E+03	2.4E+03	1.27E+04
5,5-dibutylnonane	7.63E+01	6.5E+01	4.8E+00	2.91E+02
n-nonylbenzene	2.57E+01	2.9E+01	1.3E+00	1.42E+02
1-hexadecene	2.50E+01	1.8E+01	2.2E+00	9.22E+01
n-hexadecane	2.39E+03	1.1E+03	1.4E+02	5.08E+03
fluorene	2.75E+01	3.3E+01	8.0E-01	1.56E+02
n-decylbenzene	5.30E+00	7.0E+00	0.0E+00	4.10E+01
1,4,6,7-tetramethylnaphthalene	3.90E+00	5.4E+00	0.0E+00	3.31E+01
2,6,10,14-tetramethylpentadecane(prista	1.80E+02	1.6E+02	4.9E+00	6.61E+02
hexaethylbenzene	2.00E-01	3.0E-01	0.0E+00	1.20E+00
2,6,11,15-tetramethylhexadecane	8.80E+00	1.2E+01	6.0E-01	7.54E+01
9-methylanthracene	1.00E-01	2.0E-01	0.0E+00	1.00E+00
1-phenyltridecane	1.00E+00	8.0E-01	0.0E+00	4.10E+00
pyrene	1.00E-01	4.0E-01	0.0E+00	2.40E+00

Table 4. Summary of 100 Features with the Largest Average TIC Peak Area.

Feature Number	Retention Time (min.)	Mass Spectral Identification	Mean Area%
134	34.41	n-dodecane	6.114
155	39.40	n-tridecane	5.252
81	23.42	n-decane	5.146
108	29.10	n-undecane	5.032
171	44.08	n-tetradecane	3.872
51	17.48	n-nonane	2.682
87	24.70	4-methyldecane + 1-isopropyl-3-methylbenzene	2.355
186	48.48	n-pentadecane	2.248
109	29.14	n-undecane (split peak?)	1.966
137	35.08	6-methyldodecane	1.857
150	38.04	7-methyltridecane	1.793
70	21.14	1-ethyl-3-methylbenzene or 1-ethyl-4-methylbenzene	1.759
79	23.06	1,2,4-trimethylbenzene	1.568
122	31.98	(1-methyl-1-propenyl-)-benzene	1.558
124	32.46	2-methylundecane	1.501
97	27.04	2-methyldecane	1.457
61	19.48	3-methylnonane	1.377
71	21.29	1-ethyl-2-methylbenzene	1.352
90	25.33	(1-methylpropyl-)-cyclohexane	1.326
200	60.89	d_{10}-anthracene (internal standard)	1.256
113	29.94	2-methyldecahydronaphthalene	1.216
167	43.00	2,7,10-trimethyldodecane	1.215
96	26.78	(trans)-decahydronaphthalene (isomer uncertain)	1.201
100	27.41	3-methyldecane	1.171
123	32.24	4-methylundecane	1.111
126	32.82	3-methylundecane	1.093
181	46.84	2,6,10,15-tetramethylheptadecane	0.992
95	26.65	5-methyldecane	0.972
148	37.57	2-methyldodecane	0.969
149	37.91	3-methyldodecane	0.943
72	21.56	1,2,4-trimethylbenzene or isomer	0.933
40	15.62	m&p-xylenes	0.931
115	30.52	2,8-dimethylundecane	0.917
73	21.68	3-methylnonane	0.917
117	30.84	trans-anti-1-methyldecahydronaphthalene	0.917
191	52.64	n-hexadecane	0.903
114	30.31	1-ethyl-3,5-dimethylbenzene	0.871
39	15.36	2-methyloctane	0.869
105	28.30	1-methyl-2-(1-methylethyl-)-benzene	0.848
76	22.47	1-methyl-3-propylbenzene	0.812
60	19.30	propylcyclohexane	0.798
164	42.36	2-methyltridecane	0.755
118	31.08	octylcyclohexane	0.724
88	24.98	2,6-dimethylheptane	0.705
145	37.01	6-methyldodecane	0.672
49	17.03	o-xylene	0.652
147	37.34	4-methyldodecane	0.642
67	20.69	propylbenzene	0.618

Table 4. Summary of 100 Features with the Largest Average TIC Peak Area. (Continued)

Feature Number	Retention Time (min.)	Mass Spectral Identification	Mean Area%
20	11.61	n-octane	0.617
179	46.40	cyclohexylundecane	0.604
41	15.78	3-methyloctane	0.599
139	35.49	1,2,3,4-tetrahydro-2-methylnaphthalene	0.591
103	27.96	1-methyl-2-(1-methylethyl-)-benzene	0.587
94	26.36	1-methyl-3-propylbenzene	0.551
63	19.93	4-(1-methylethyl-)-heptane or 3-ethyl-2-methylheptane	0.527
56	18.69	4,5-dimethylcyclohexen-1-one	0.501
75	22.23	(1-methylethyl-)-benzene	0.488
131	33.82	naphthalene	0.484
47	16.76	trans-1-ethyl-4-methylcyclohexane	0.463
119	31.25	decylcyclopentane	0.452
102	27.86	2-ethyl-1,4-dimethylbenzene	0.450
57	18.93	4-methylnonane	0.449
99	27.29	1-methyl-2-propylbenzene	0.398
93	26.12	citronella (?)	0.397
104	28.14	2,3-dihydro-2-methyl-1H-indene	0.393
174	44.77	2,6-dimethylnaphthalene	0.375
106	28.47	2,3-dihydro-1-methyl-1H-indene	0.374
62	19.84	2-ethyl-1,3-dimethylcyclohexane	0.366
69	21.03	5-methylnonane	0.358
158	40.39	1-methylnaphthalene	0.353
53	17.92	trans-1-ethyl-4-methylcyclohexane	0.339
55	18.49	nonadecanoic acid, hexyl ester (not very likely)	0.335
68	20.89	1,1,2,3-tetramethylcyclohexane	0.296
2	5.23	cyclohexane + benzene	0.294
85	24.19	C15-hydrocarbon	0.291
7	7.68	4,4-dimethyl-2-pentene	0.287
140	35.75	unidentified	0.281
195	56.60	n-heptadecane	0.278
130	33.69	2,3,6-trimethyldecane	0.278
31	13.76	1,1,3-trimethylcyclohexane	0.276
163	42.12	4,5-dimethylnonane	0.270
46	16.61	1-methyl-2-propylcyclopentane	0.266
37	14.87	2,3-dimethylheptane	0.265
77	22.63	cis-octahydro-1H-indene	0.262
166	42.69	3-methyltridecane	0.260
74	21.88	6-methyl-4-decene	0.260
91	25.54	2,3-dihydro-1H-indene	0.253
162	41.89	unidentified branched hydrocarbon	0.250
28	13.25	2,6-dimethylheptane	0.234
146	37.06	2,6-dimethylundecane	0.227
15	10.44	1,4-dimethylcyclohexane	0.224
36	14.62	unidentified	0.224
48	16.88	1-ethyl-4-methylcyclohexane	0.223
161	41.61	(1-methylethyl-)-cyclohexane	0.221
30	13.56	ethylcyclohexane	0.220
98	27.18	citronella	0.213
13	9.77	toluene	0.206
152	38.70	7-methyl-6-tridecene	0.203

Table 4. Summary of 100 Features with the Largest Average TIC Peak Area. (Continued)

Feature Number	Retention Time (min.)	Mass Spectral Identification	Mean Area%
38	15.14	ethylbenzene	0.199
159	40.65	3-methylheptane	0.185

SECTION VI

CONCLUSIONS

The sample set collected with the aid of the Defense Logistics Agency, probably represents a reasonable sampling of JP-8 fuel as it may be encountered worldwide. Statistical values from this sampling should be useful in predicting the overall JP-8 population. The average concentration of each compound, listed in column 2 of Table 3 can be treated as the expected or typical concentration for that compound in JP-8. The maximum detected concentration for each compound, listed in column 5 of Table 3 can be treated as the upper bound for the compound's concentration in JP-8 for environmental release calculations.

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